Driven classical diffusion with strong correlated disorder

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We analyze one-dimensional motion of an overdamped classical particle in the presence of external disorder potential and an arbitrary driving force F. In thermodynamical limit the effective force-dependent mobility $\mu(F)$ is self-averaging, although the required system size may be exponentially large for strong disorder. We calculate the mobility $\mu(F)$ exactly, generalizing the known results in linear response (weak driving force) and the perturbation theory in powers of the disorder amplitude. For a strong disorder potential with power-law correlations we identify a non-linear regime with a prominent power-law dependence of the logarithm of $\mu(F)$ on the driving force.

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We consider stationary diffusion in one dimension (1D), in the presence of a random disorder potential and a constant driving field. We show that the effective field-dependent mobility $\mu(F)$ is self-averaging, and calculate its dependence on the field F for various forms of correlated disorder. In particular, for a stationary diffusion in a strong disorder potential with power-law correlations at large distances [Eqs. (5), (11)], there is a wide intermediate range of values of the driving force F where the logarithm of the effective mobility scales as a non-trivial power of F (Fig. 1). With Coulomb-like ($n = 1$) or longer-range correlations, the effective mobility is a singular function of F already at $F = 0$; the applicability region of the linear transport is essentially absent (Fig. 2). These properties remain in the presence of weak interaction between the particles, introduced here at the level of the self-consistent Poisson equation which describes a Debye-like screening in the presence of strong disorder.

Our results apply to a number of systems where classical diffusion[1,2,3,4] is the main mechanism of transport. Other applications include carrier diffusion in semiconductor nanostructures, nano-scale thermoelectrics[5,6], transport in DNA[7] and other biological systems. In particular, the mean-field interaction model is directly applicable to ionic transport through cell membranes[8], where one expects a number of parallel identical channels.

Single-particle diffusion in 1D is described by the Smoluchovsky equation

$$\eta_0 \dot{x} + \partial_x U(x) = f(t), \tag{1}$$

where $U(x)$ is the external potential and $f(t)$ is the thermal force with the correlator $\overline{f(t)f(t')} = 2T\eta_0\delta(t-t')$. The usual assumption is that the bare viscous friction coefficient η_0 is determined by fast scattering events off phonons, short-range disorder, etc. The potential $U(x)$ in Eq. (1) is thus the part of the overall potential remaining after averaging over some distance scale; its precise value depends on the specific physical system. If we assume the carriers have charge e, we can also define the bare mobility in the absence of disorder, $U(x) = -eEx$:

$$\mu_0 \equiv \overline{\dot{x}}/E = e/\eta_0. \tag{2}$$

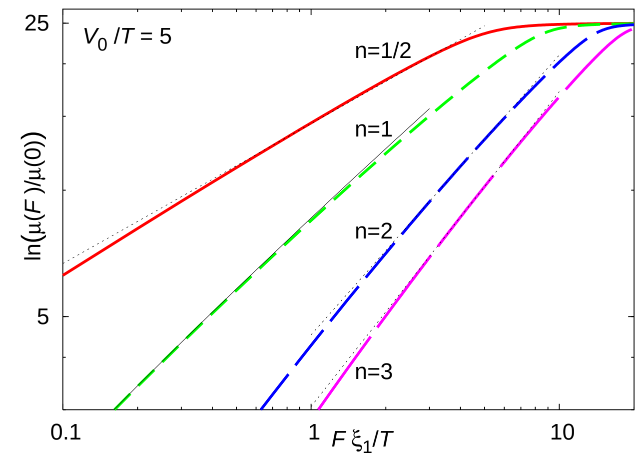

FIG. 1: Logarithm of the effective mobility renormalization $\ln\bigl(\mu(F)/\mu(0)\bigr)$ [Eqs. (6), (7)] with the correlation function $g(x) = (1 + x^2/\xi_1^2)^{-n/2}$ for strong disorder ($V_0/T = 5$) and large driving forces F. Dotted lines guide the eye with the slope of the intermediate asymptote (14). Thin solid line is the analytic result (15) for $n = 1$.

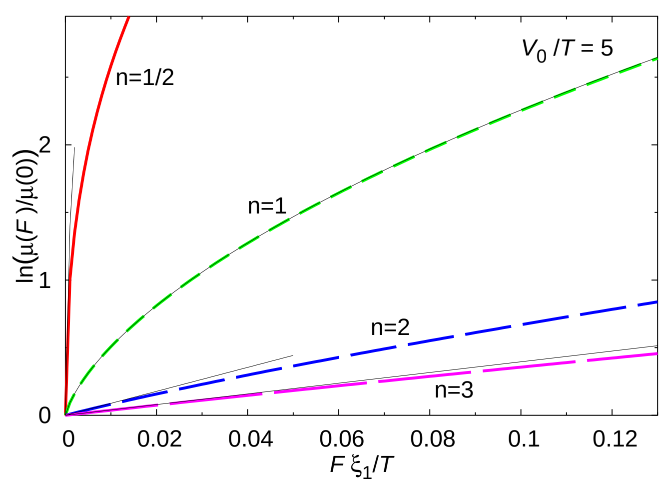

FIG. 2: As in Fig. 1 but for small driving forces F. Thin solid lines indicate the non-linear correction calculated analytically: linear in F for $n > 1$, proportional to F^n for $n < 1$, and Eq. (15) for $n = 1$.

The equation (1) can be also rewritten as the transport equation for the average particle density $n \equiv n(x,t)$ and the particle current $j \equiv j(x,t)$,

$$\partial_t n + \partial_x j = 0, \quad j = -D_0 \partial_x n - \eta_0^{-1} n\, \partial_x U(x); \tag{3}$$

the diffusion constant D_0 is related to the viscous friction coefficient η_0 by the Einstein relation, $D_0 = T/\eta_0$.

The usual transport problem corresponds to stationary diffusion in the presence of a random Gaussian potential $V(x)$ and a constant driving force F, with the total potential energy $U(x) = V(x) - Fx$. In the case of a periodic potential $V(x) = V(x+a)$, the stationary solution[1,2,3] corresponds to a constant average current j with periodic boundary conditions, $n(a) = n(0)$. Then, by normalizing the density profile $n(x)$ over the period, we can use the current to define the average drift velocity, $\bar{v} = j/\bar{n} = ja$, as well as the effective viscous friction coefficient $\eta \equiv F/\bar{v} = F/ja$,

$$\eta = \frac{\eta_0 F}{aT} \int_0^a dx \int_x^{x+a} dx' \, \frac{e^{[V(x') - V(x) + F(x-x')]/T}}{1 - e^{-Fa/T}}. \tag{4}$$

Both integrations extend over the entire period, and, as it often happens in classical transport phenomena, for a sufficiently large a the effect of disorder becomes self-averaging [the required size can be large, see Eq. (20) below]. In such cases we can replace Eq. (4) by its average over disorder. We assume that the disorder distribution is Gaussian with the correlations

$$\langle V(x) \rangle = 0, \quad \langle V(x) V(x') \rangle = V_0^2 g(x - x'), \tag{5}$$

where the local r.m.s. value V_0 is taken as the measure of the disorder strength and the correlation function $g(x)$ is defined so that $g(0) \equiv 1$. Then, in the thermodynamical limit $a \to \infty$, the effective mobility $\mu(F) \equiv e/\langle \eta \rangle$, and

$$\frac{\mu_0}{\mu(F)} = e^{V_0^2/T^2} \frac{F}{T} \int_0^\infty dx \, e^{-Fx/T} \, e^{-g(x) V_0^2/T^2}, \;\; F > 0. \tag{6}$$

In the small-F limit (but at the same time $aF \gg T$), this gives the usual linear response result[9,10,11,12],

$$\langle \eta \rangle / \eta_0 \overset{F \to 0}{=} \mu_0/\mu(0) = \exp(V_0^2/T^2), \tag{7}$$

which can be understood as the average of the activation exponent of the difference between the highest maximum and the lowest minimum of the potential. Generically, these would be in different parts of the sample and so the friction renormalization factors onto a product of the two averages $\langle e^{V/T} \rangle \langle e^{-V/T} \rangle = \exp(V_0^2/T^2)$, independent of the form of the correlation function $g(x)$.

Similarly, the stationary limit of the dynamical perturbation theory[13,14] is restored by expanding Eq. (6) in powers of V_0/T and integrating the result by parts,

$$\frac{\mu_0}{\mu(F)} = 1 - \frac{V_0^2}{T^2} \int_0^\infty dx \, e^{-Fx/T} \, g'(x) + \mathcal{O}(V_0^4/T^4). \tag{8}$$

The disorder correlation function $g(x)$ is expected to decrease with x, remaining substantially different from zero over the distance of the order of the appropriate correlation length ξ. It is clear from the weak-disorder expression (8) that for such finite-range disorder there is a distinct crossover force $F_\xi \sim T/\xi$: while $F \lesssim F_\xi$ have relatively little effect on the mobility, larger values of F begin to suppress the effect of disorder as large-scale potential valleys and hills gradually disappear.

To analyze an analogous effect for *strong* finite-range disorder, note that for large V_0/T, $\Delta_x \equiv e^{-g(x) V_0^2/T^2}$ is exponentially small for $x \lesssim \xi$. This effectively limits the integration in Eq. (6) to the region $x \gtrsim \xi$, so that

$$\ln\bigl(\mu(F)/\mu(0)\bigr) \sim F\tilde{\xi}/T, \tag{9}$$

where $\tilde{\xi} \approx \xi$ up to a logarithmic correction. Such a dependence on the applied field is analogous to the logarithmic susceptibility[15] typical for systems with activated transport. Here it can be understood as the diffusion limited by far-spaced maxima of the potential, with the particles concentrated in the intermediate low minima; the applied driving force F effectively reduces the energy gap between the minima and the maxima and therefore has an *exponential* effect on the mobility.

The expression (9) is valid qualitatively as long as the effect of the disorder remains large, $\mu_0/\mu(F) \gg 1$. The precise value of $\tilde{\xi}$ and the prefactor depends on the details of the disorder correlation function. For example, with the exponential correlation function $g(x) = \exp(-x/\xi)$, the integration (6) can be done exactly in terms of the incomplete gamma function; the asymptotic form for $V_0^2/T^2 \gg \max(1, \chi \equiv F\xi/T)$ is

$$\frac{\mu(F)}{\mu(0)} = \frac{(V_0/T)^{2\chi}}{\Gamma(\chi+1)} \overset{\chi \gtrsim 1}{\to} (2\pi\chi)^{-1/2} \, e^{F\tilde{\xi}/T}, \tag{10}$$

where $\tilde{\xi} = \xi\bigl[1 + \ln\bigl(V_0^2/(TF\xi)\bigr)\bigr]$.

The disorder-induced transport non-linearity becomes even more pronounced for long-range potentials, e.g., those with power-law correlations at large distances. With long-range correlations the far-spaced maxima and minima of the potential are not entirely independent and, therefore, even a weak driving force may have a noticeable effect. Specifically, consider a correlation function with the asymptotic form

$$g(x) = (\xi_1/x)^n, \quad x > x_{\min} \gg \xi, \xi_1. \tag{11}$$

With strong enough disorder $[g(x_{\min}) V_0^2/T^2 \gtrsim 1]$ the integral (6) will be determined by large x, in which case the expression can be rewritten approximately as

$$\frac{\mu(0)}{\mu(F)} \approx \mathcal{I}_n(\alpha), \;\; \mathcal{I}_n(\alpha) \equiv \int_0^\infty dx \, e^{-x - \alpha x^{-n}}, \tag{12}$$

where $\alpha \equiv \bigl(F\xi_1/T\bigr)^n V_0^2/T^2$ can be small or large within the strong-disorder domain where Eq. (12) is applicable.

For sufficiently large α, the integration can be done using the Gaussian approximation around the maximum at $x_0 = (n\alpha)^{1/(n+1)}$,

$$\mathcal{I}_n(\alpha) = \left(\frac{2\pi x_0}{n+1}\right)^{1/2} e^{-x_0(1+1/n)}, \ \ \alpha \gtrsim 1. \qquad (13)$$

As a result, logarithm of $\mu(F)$ is proportional to a power,

$$\ln\bigl(\mu(F)/\mu(0)\bigr) \sim \bigl(F\tilde{\xi}_1/T\bigr)^{n/(n+1)}, \qquad (14)$$

with a *large* temperature-dependent length parameter $\tilde{\xi}_1 = C_n \xi_1 \,(V_0/T)^{2/n}$, $C_n \equiv (n+1)^{1+1/n}/n$ [cf. Eq. (9)]. For small $\alpha \ll 1$, the integration (12) can be done perturbatively in powers of $\alpha \propto F^n V_0^2$ for $n<1$ or, using the identity $\mathcal{I}_n(\alpha) = \mathcal{I}_{1/n}(\alpha^{1/n})$, in powers of $\alpha^{1/n} \propto F V_0^{2/n}$ for $n>1$. For Coulomb disorder, $n=1$, the result is expressed in terms of the Macdonald function,

$$\mu(0)/\mu(F)\big|_{n=1} \approx \mathcal{I}_1(\alpha) = 2\alpha^{1/2} K_1(2\alpha^{1/2}). \qquad (15)$$

For very small $\alpha \ll 1$, $\mathcal{I}_1(\alpha) \approx 1 - \alpha \ln\bigl(e^{1-2\gamma}/\alpha\bigr)$, where $\gamma \approx 0.577$ is the Euler's constant; the correction is linear in F up to a logarithm. Clearly, for strong Coulomb or longer-range disorder, $n \le 1$, the mobility $\mu(F)$ is a singular function of the driving force at $F=0$; the linear-transport regime is essentially absent. These asymptotics are illustrated in Figs. 1, 2 for a model form of the disorder correlation function $g(x) = (1 + x^2/\xi_1^2)^{-n/2}$.

Self-averaging. Our conclusions on the scaling of mobility in strongly-disordered diffusive 1D systems are based on the average, Eq. (6). To analyze the sample-to-sample fluctuations, consider the irreducible average $\langle\!\langle \eta^2 \rangle\!\rangle \equiv \langle \eta^2\rangle - \langle \eta\rangle^2$ of the effective friction η [Eq. (4)],

$$\frac{\langle\!\langle \eta^2 \rangle\!\rangle}{\eta_0^2} = e^{2V_0^2/T^2} \frac{F^2}{a\,T^2} \int_0^a\! dx\, e^{-Fx/T} \Delta_x \int_0^a\! dy\, e^{-Fy/T} \Delta_y \times \int_0^a\! dz \left(\Delta_{z+\frac{x+y}{2}} \Delta_{z-\frac{x+y}{2}} \Delta^{-1}_{z+\frac{x-y}{2}} \Delta^{-1}_{z-\frac{x-y}{2}} - 1\right), \qquad (16)$$

where the correlator $\Delta_z \equiv e^{-g(z)V_0^2/T^2}$ is periodic under $z \to z+a$. Note that both Δ_z and Δ_z^{-1} enter Eq. (16). Therefore, unlike in the average (6), both short- and long-distance disorder correlations affect the variance of η.

For weak disorder, the expansion of Eq. (16) in powers of $V_0/T \ll 1$ begins with the quartic term,

$$\begin{aligned}\frac{\langle\!\langle \eta^2 \rangle\!\rangle}{\eta_0^2} &= \frac{V_0^4}{T^4}\frac{F^2}{aT^2} \int_0^a\! dx\, e^{-Fx/T}\! \int_0^a\! dy\, e^{-Fy/T}\! \int_0^a\! dz \\ &\quad \times g_z \left(2g_z + g_{z+x+y} + g_{z+x-y} - 2g_{z+x} - 2g_{z+y}\right) \\ &= \frac{2V_0^4}{aT^4} \int_0^a\! dz\, g_z \!\int_0^a\! du\, e^{-Fu/T}\,(u g''_{z+u} - g'_{z+u}). \end{aligned} \qquad (17)$$

The integration is simplified in the limits of weak and large F; the combined result is

$$\frac{\langle\!\langle \eta^2 \rangle\!\rangle}{\eta_0^2} = \frac{V_0^4}{2aT^4} \min(4\xi_2, T/F), \ \ \xi_2 \equiv \int_0^\infty\! dx\, g^2(x). \qquad (18)$$

Here, ξ_2 is yet another correlation length, finite for short-range disorder and for long-range disorder with $n > 1/2$. Clearly, for weak disorder the variation of η is small and it is further reduced with increasing system size a.

The situation is different for strong disorder, $V_0 \gg T$, which causes an exponential renormalization of η; large fluctuations are also expected. In this case Δ_x^{-1} has a prominent maximum at the origin. Consequently, the integral (16) gets an exponentially large contribution from a vicinity of the point $z=0$, $x=y$. Using the steepest descent method, we obtain

$$\frac{\langle\!\langle \eta^2 \rangle\!\rangle}{\eta_0^2} = \frac{2\pi F^2 e^{4V_0^2/T^2}}{aV_0^2} \int_0^\infty\! du\, \frac{e^{-2Fu/T} e^{-4g(u)V_0^2/T^2}}{g''(u) - g''(0)}. \qquad (19)$$

For not exceedingly large F the result is determined by values of u away from the origin. Then, the denominator can be replaced by a constant[18] $-g''(0) \equiv 2/\xi_0^2$, and the integral acquires precisely the form of Eq. (6). Generally,

$$\frac{\delta\mu^2}{\mu^2} \approx \frac{\langle\!\langle \eta^2 \rangle\!\rangle}{\langle\eta\rangle^2} = C\, \frac{\pi F\, T \xi_0^2}{2a\, V_0^2}\, e^{2V_0^2/T^2}; \qquad (20)$$

while F in the prefactor can be small, it is assumed to be large on the scale of the system size, $Fa/T \gg 1$. The normalization in Eq. (20) is chosen so that for short-range disorder $C \approx 1$ [cf. Eq. (9)]. For power-law correlation tail, $C = \mathcal{I}_n(2^{n+2}\alpha)/[\mathcal{I}_n(\alpha)]^2$, with $\alpha \equiv (F\xi_1/T)^n V_0^2/T^2$ [cf. Eqs. (11), (12)]. Overall, we conclude that the effective mobility is a self-averaging quantity in the thermodynamical limit. Of course, the required system size can be large if the fluctuations are strong.

We verified these conclusions by simulating diffusion in a 1D short-range random potential (not shown). With periodic boundary conditions the viscous friction (4) could be obtained by averaging the time t it takes a particle to travel over one period, $\Delta x = a$. As expected, with increasing a, the corresponding disorder average $\langle t\rangle/a$ approached the inverse of the average drift velocity.

Stationary diffusion with weak interaction. The considered problem differs from the canonical Kramers problem[1,2,3] of over-the-barrier transport, where it is the dynamical equilibrium that establishes the exponentially different particle numbers in the "reservoirs" on the two sides of the barrier. Here, we consider a situation corresponding to a typical resistivity measurement in a macroscopic sample where the total number of particles does not change with the applied field. Then, the macroscopic current would be determined solely by the average drift velocity. It is important that the quantity is self-averaging, as the explicit disorder averaging would not be necessary for large enough samples. Previously, stationary driven diffusion was considered within the linear response with random disorder[9,10,11,12], and also for arbitrary F in *deterministic* periodic potentials[2,3,16,17].

In finite-size systems such a situation arises naturally, e.g., when diffusing particles are charged and the electroneutrality condition needs to be satisfied. The simplest case corresponds to the Debye mean-field screening, where the potential in Eq. (3) is modified by the

self-consistent potential, $U(x) \to U(x) + e\varphi(x)$. Specifically, we consider a 1D Poisson equation,

$$\varphi'' = -4\pi e(n - \bar{n}), \tag{21}$$

as would be appropriate for diffusion in a 3D system with 1D-modulation (layered disorder), a parallel bunch of identical DNA molecules, or electrostatically-coupled ionic cell channels.

In the static equilibrium, $F = 0$, the coupled Eqs. (3), (21) correspond to the non-linear screening problem; with weak disorder, $V_0 \ll T$, the Debye screening length is κ^{-1}, $\kappa^2 \equiv 4\pi\bar{n}e^2/T$. The linearized self-consistent screening problem can be also solved with the non-zero driving force, $F > 0$; the solution involves two screening parameters, $s_\pm = (\kappa^2 + f^2/4)^{1/2} \pm f/2$, where $f \equiv F/T \approx j/(D_0\bar{n}) \equiv \lambda$. Clearly, in the weak-interaction limit, $f \gg \kappa$, the shorter screening length $s_+^{-1} \approx f^{-1} = T/F$ is determined by the driving force, while the longer one diverges, $s_-^{-1} \approx f/\kappa^2$.

With the driving force and a strong disorder, the problem is forbiddingly complicated. However, if the interaction is weak, the additional potential would be small, and the screening equations can be linearized. To this end, it is convenient to eliminate the density n from Eqs. (3), (21) and write the self-consistent equation for the scaled gradient of the screening potential $\varepsilon \equiv e\varphi'(x)/T$,

$$\varepsilon'' + \varepsilon'\Big(\frac{V'}{T} - f\Big) - \kappa^2\varepsilon = \tau - \varepsilon\varepsilon',\ \tau \equiv \kappa^2\Big(\frac{V'}{T} + \lambda - f\Big).$$

This equation can be rewritten identically as

$$e^{-V/T}\Big(\frac{d}{dx} - s_+\Big)e^{V/T}\Big(\varepsilon' + s_-\varepsilon\Big) = \tau - \Big(\varepsilon' - s_-\frac{V'}{T}\Big)\varepsilon.$$

For weak interaction, the last term in the r.h.s. is quadratic in small κ^2 and can be ignored. The remaining equation should be solved for ε with zero boundary conditions at infinity. The relation between the driving force $F \equiv fT$ and the diffusion current $j \equiv \lambda\bar{n}D_0$ is established from the self-consistency condition that the screening does not modify the net driving field. Equivalently, the disorder-averaged $\langle\varepsilon\rangle = 0$. Approximating $s_+ \approx f$, after some algebra we again arrive at Eq. (6).

Conclusions. We analyzed the stationary 1D problem of a driven diffusion in the presence of a random disorder potential. For large systems and/or in the presence of an interaction fixing the number of particles transport should be described in terms of the effective mobility μ. Strong disorder significantly reduces the mobility and leads to its non-trivial scaling as a function of the driving field F and the temperature. With finite-range disorder, the dependence $\mu(F)$ can be described in terms of the logarithmic susceptibility, Eq. (9), a generic form for problems with activated transport. For a strongly-driven system with power-law disorder correlations the logarithm of the mobility scales as a power of the driving force, Eq. (14). The disorder effect is especially pronounced for Coulomb-like correlations [see Eq. (15)]: the field-dependent correction to mobility is singular already at $F = 0$.

The obtained explicit results are applicable for a number of systems where diffusion is the main transport mechanism, and can be especially useful for characterization of disorder distribution. Both quantum effects and particle-particle interaction would further modify the functional form of mobility. For the purposes of comparison with experiment at low temperatures, it would be useful to obtain the corresponding results beyond the usual asymptotic limits of zero temperature and delta-correlated disorder.

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18. Here ξ_0 is a correlation length describing the short-distance properties of the disorder potential; it may be quite different from the length ξ relevant at large distances.